LETTERS TO THE EDITOR

To the Editor:

Two recent papers (Sood et al., 1979; Sood and Reklaitis, 1979) have again drawn attention to the power and utility of linear equation methods in connection with material balance calculations. In an appendix to their first paper, concerned with the unconstrained case, they point out a familiar problem to users of linear equation methods. Some formulations of recycle problems lead to situations which cannot be solved.

In the general simultaneous method (Hutchison, 1974) a properly adapted equation solving method can obtain perfectly correct partial solutions to these situations, and can report the offending components as "undetermined" in, and downstream of, any recycle loops in which they occur. The reason for the occurrence of such situations, is, as suggested (Sood et al., 1979) that inadequate steps have been taken to define the flow of the offending component in the loop or loops concerned.

To assist in the recognition of this situation when the problem is being set up, use may be made of a "rule of escape" formulated some years ago (Anon. 1973) by the writer.

Rule of Escape: "If, in a process, any component can find its way into a loop, then somewhere there must be a route for it to escape from the loop, in which the rate of escape, by reaction or by separation, must be related to the amount of that component in the loop."

The mathematical analysis of the situation by Sood et al. (1979) is perfectly correct, but is of little use in avoiding the problem. The proper application of the Rule of Escape will lead to the recognition of all cases in which the situation can arise, either in their method or in the general simultaneous method.

It is also a useful rule of thumb for avoiding accumulation of trace materials in real recycle situations.

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LITERATURE CITED

Anon., "SYMBOL User's Manual" Computer Aided Design Centre, Madingley Road, Cambridge (1973).

Hutchison, H. P., "Plant Simulation by Linear Methods," *Trans. Instn. Chem. Engrs.*, **52**, 287 (1974).

Sood et al., "Solution of Material Balances for Flowsheets Modeled with Elementary Modules: The Unconstrained Case," *AIChE J.*, **25**, 209 (March, 1979).

Sood, M. K., and G. V. Reklaitis, "Solution of Material Balances for Flowsheets Modeled with Elementary Modules: The Constrained Case," *AIChE J.*, **25**, 220 (March, 1979).

Reply:

H. P. Hutchison's Rule of Escape is a welcome addition to the analysis of material balance problems. As Mr. Hutchison suggests, it certainly is possible to identify undetermined components or dependent specifications during the solution process. The program MBP-II implementing the methods described in our papers, in fact, does perform this identification.

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To the Editor:

I would like to make some comments about the results presented by Ruschak [*AIChE J.*, **24**, 705 (1978)] for the flow of a falling film into a pool. The Reynolds number in Ruschak's work is defined according to Nusselt's classic work as $R = 3\rho Q/\mu$. Since the flow rate Q is a function of the upstream film thickness D, $R = \rho^2 GD^3/\mu^2$. Obviously, a zero Reynolds number may only correspond to a zero film thickness, that is a zero flow rate. However, Ruschak displays in his Figure 1, a complete fluid surface with finite film thickness for this case $R = 0$, and claims that the solution is particularly "exact" in this case. In Figure 2 he displays a complete analysis of the minimum and maximum film thickness for the same $R = 0$. Another comment is with regard to a film thickness parameter $d = D/C$ introduced by the author. According to his definitions, obviously, there is a correlation between, this parameter and the Reynolds number, namely $d = R^{1/3}\ (\mu/\rho G^{1/2})^{2/3}/C$. Subsequently, arbitrary values for both d and R may not be assigned. However, we find that the author did vary both parameters as independent variables. For instance, in Figures 1 and 2, the zero Reynolds number is investigated for a wide range of d values ($10^{-5} \leq d \leq 10^{-1}$) in violation of the mentioned d and R correlation. One should not forget that the author has based his analysis on C and $\rho GD^2/\mu$ as characteristic values for distance and velocity respectively. Therefore, these values are assumed to be finite. Another point should be raised about the obscurity of what Ruschak calls the static meniscus parameter α. Integration of the capillary hydrostatics equations yields $\alpha = [h_{xx}(1 + h_x^2)^{-3/2}]^2 + 2h_x(1 + h_x^2)^{-1/2}$ which includes an arbitrary constant α. This equation is used by Ruschak as a boundary condition for the static meniscus, that is the stagnant fluid surface in the pool. Obviously one would expect a stagnant fluid surface in a large pool to be horizontal, and accordingly at this surface $h_x \rightarrow \infty$, and $h_{xx} = 0$ which leads to $\alpha = 2$. Any other value for α would be the result of a different combination of h_x and h_{xx} values at the stagnant surface of the pool, which undoubtedly would imply a non-horizontal stagnant fluid surface (inclined or curved). Since most of Ruschak's results are displayed for a complete range of α values ($0.1 < \alpha < 100$), the obvious implication is that the stagnant fluid surface in a large pool is not necessarily horizontal. Although Ruschak reports that above the transition region his calculations revealed a series of standing waves he did not give any detail about these waves especially their wavelengths as compared to the wavelength of the prominent ripple reported. As reported by Cook and Clark [*Ind. Eng. Chem. Fundam.*, **12**, 1 (1973)], these standing short wavelength waves were observed in the presence of a stagnant surfactants band and may be produced by a fine needle which was allowed to touch the surface of the falling liquid film. In both cases these ripples are the result of a localized pressure change on the surface of a flowing liquid and were not observed in the absence of this pressure. Cook and Clark found that their wavelength was of order of magnitude of 1 mm, while the length of the prominent ripple was about 1-4 cm. Wilkes and Nedderman [*Chem. Eng. Sci.*, **17**, 177 (1962)] mentioned the disparity in wavelengths obtained by an equation similar to that used by Ruschak and their experimental measurements of the series of ripples. The apparent reason for the failure to theoretically simulate these ripples is that the stagnant band of surfactants was not included in either Wilkes and Nedderman equation or that of Ruschak. The standing waves reported by Ruschak should not be confused with those observed above the stagnant band or in the fine needle case. They are probably a result of the mathematical disturbance induced as an initial condition for the differential equation to deviate the solution from Nusselt's constant film thickness case. Moreover, the method used by Ruschak is based on small surface slope, which obviously limits the solution to long wavelength waves and can not produce short ripples without violating this basic assumption. A comment about the mathematical consistency of Ruschak's approximation should be made. The method of approximation is based on the assumption that the surface slope $\|h_x\| << 1$ is small, and terms evaluated as h_x^2 or smaller were neglected. Ruschak applied the approximation to the final stage and then suddenly changed the rules and included h_x^2 in the curvature term K. If terms of the order $O(h_x^2)$ were important then for example, the boundary condition $u_y = 0$ should have been $u_y(1 - h_x^2) + u_x = 0$, instead and this would have contributed to a considerable change in the results.

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Reply:

The criticisms by Esmail of the paper "Flow of a Falling Film into a Pool" are rejected. Esmail does not contest the main result of the paper, which is a mechanism for the rapid thinning of a liquid film where it enters a pool. The insight is useful, as the phenomenon occurs in many flows. Recently, Jones and Wilson [*J. Fluid Mech.*, **87**, 263 (1978)] found the phenomenon to be important in bubble coalescence and arrived at the same mechanism.

Contrary to Esmail's claim, the two dimensionless groups employed in the paper, namely the Reynolds number, R, and the ratio of the film thickness far upstream to the capillary length, d, are independent. The flow has five independent parameters (ρ, μ, σ, G, and D) from which two independent dimensionless groups can be formed. Given only R, d cannot be calculated. Indeed this is obvious, as d involves surface tension whereas R does not.

The exact solution given to the approximate governing equation at zero Reynolds number is applicable on an interval of Reynolds number about zero. The region of applicability was determined by finding the first effects of increasing Reynolds number. It is difficult to see what confuses Esmail about this standard approach.

The concept of a pool of liquid, as used in the paper, implies that the region into which the film flows, whether bounded or unbounded in extent, may be regarded as motionless. It certainly does not imply that the interface is ultimately horizontal. If the film thickness far upstream is much less than the characteristic dimension of the region into which the film flows, then that region is, relative to the film, a pool. Flow at the rear of a long bubble rising through a slot is one example where the interface is not ultimately horizontal.

Esmail is stating the obvious when he points out that the paper is not about the ripples above a stationary surface film which is parallel to the wall or about those produced by a fine needle. As even the title of the paper makes plain, the analysis applies where a liquid layer flows into a relatively large reservoir. Regardless of whether a stationary surface film is present, the pressure in the liquid drops from atmospheric where the flow parallels the wall to below atmospheric in the reservoir near the wall where the meniscus is curved. The viscous dissipation of this pressure drop gives rise to film thinning and ripples above the reservoir, as explained in the paper.

The mathematical analysis employed is consistent provided that it is verified a posteriori that dynamic effects in the liquid layer become negligible while the slope of the interface is still small. This was the case for the results presented.

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To the Editor:

We believe that the following corrections are necessary in the paper of Bhavaraju et al. (1978).

In Part I (p. 1063),

1) Equation (25) should read

$$\gamma_0 = \sigma^2(1 + H)$$

2) Equation (47) should read

$$\tilde{\tau}_{rr}|_{\tilde{r}=R} = \sigma^{2m}[2\cos\theta + m(-7.6\cos\theta + 9.1\cos^3\theta - 3.1\cos^5\theta + 1.5\cos^7\theta)]$$

3) In Equation (51), the exponent of 2 should be $2m$ rather than m.

4) In Fig. 2, the scale of the ordinate goes from 1.0 to 2.0.

In Part II (p. 1070), by examining the dissertation of Bhavaraju (1978), the following corrections appear to be necessary in order that Equations (13) thru (16) would yield results that agree with those in Fig. 2.

1) In Equations (13) and (14) the denominators should read $1 - \phi^{-(2n+3)/3}$ rather than $1 - \phi - (2n+3)/3$.

2) In Equation (15), the first term on the right hand side should read

$$\frac{6n(n-1)}{(2n+1)(1-\phi^{1/3})}$$

rather than

$$\frac{6n(n-1)}{(2n+1)(1-\phi^{1/3})^2}$$

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LITERATURE CITED

Bhavaraju, S. M., "Mass transfer in simple and viscous gas-liquid contactors for fermentation processes," Ph.D. dissertation, Univ. Microfilms Internatl., Ann Arbor, Michigan (1978).

Bhavaraju, S. M., R. A. Mashelkar, and H. W. Blanch, "Bubble Motion and Mass Transfer in non-Newtonian Fluids," *AIChE J.*, **24**, 1063 and 1070 (1978).

ERRATA

In the Letters to the Editor section [*AIChE J.*, **26**, 334 (1980)] the address for R. G. Rice should read: Chemical Engineering Department, Montana State University, Bozeman, Montana 59717.

In "Bubble Motion and Mass Transfer in Non-Newtonian Fluids," by Bhavaraju, S. M., Mashelkar, R. A., and Blanch, H. W., *AIChE J.* **24** Part I, 1063, Part II, 1070, the following should read:

Part I

Equation (25)

$$\gamma_0 = \dot{\sigma}^2(1 + H)$$

Equation (47)

$$\tilde{\tau}rr|_{\tilde{r}=R} = \sigma^{2m}[2\cos\theta + m(-7.6\cos\theta + 9.1\cos^3\theta - 3.1\cos^5\theta + 1.5\cos^7\theta]$$

Equation (51)

$$F^D(m) = 3^m 2^{2m}(1 - 7.66\text{m})$$

Part II

Equation (13), (14)—denominators should read $[1 - [\phi^{-2n+3)/3}]$

Equation (15) right hand side should read

$$\frac{6n(n-1)}{(2n+1)(1-\phi^{1/3})}$$

In "Restrictions and Equivalence of Optimal Temperature Policies for Reactors with Decaying Catalysts" by J. M. Pommersheim, L. L. Tavlarides and S. Mukkavilli [*AIChE, J.*, **26**, 327 (1980)] a number of corrections of typographical errors which were made by the authors in the galleys were not executed prior to printing. The corrections follow:

p 327, column 2, line 1; "to the" should read "to be".

p 327, column 2, line 3; "Equation" should read "Equations".

Equation (6); "dg_k" should read "dy_k".

p 328, column 1, line 1; "$\partial\psi$" should read "$d\psi$".

p 328, column 1, line 22; "$E_D > E_R$" should read "$E_D < E_R$".

Equation (11); "E_r" should read "E_R".

Equation (26); "$\left(\frac{\partial F}{\partial \dot{y}_{k-}}\right) = \left(\frac{\partial F}{\partial \dot{y}_{k+}}\right)$"

should read "$\left(\frac{\partial F}{\partial \dot{y}_k}\right)_- = \left(\frac{\partial F}{\partial \dot{y}_k}\right)_+$".

p 329, column 2, line 42; "Litmann" should read "Leitmann".

p 330, column 1, line 8; "rate constant for deactivation reaction" should read "frequency factor for reaction."

p 330, column 1, line 15; "∂_y" should read "∂y".